Discovering Hidden Geothermal Signatures using Unsupervised Machine Learning

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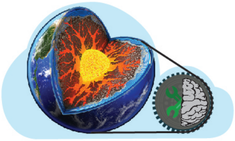
`http://tensors.lanl.gov`

Support: (1) DOE Geothermal Technologies (GTO), Machine Learning for Geothermal Energy
(2) LANL LDRD DR, Unsupervised Machine Learning
LA-UR-20-21322

NMFk



NTFk

Machine Learning (ML) methods

- **Supervised** ML: learns everything from data
  ⇒ requires big training datasets
  ⇒ highly sensitive to data noise (adversarial examples)
  ⇒ cannot discover something that we do not know already
- **Physics-informed** ML: learns from data but includes preconceived knowledge about the governing processes
  ⇒ requires smaller training datasets
  ⇒ produces better predictability with lower uncertainty
  ⇒ robust to data noise
- **Unsupervised** ML: extracts features from data (features characterizing data variability)
  ⇒ unbiased analyses not impacted by data labeling, subject-matter expertise, and physics assumptions

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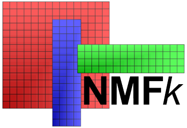
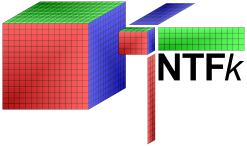
Unsupervised Machine Learning Applications

- **Feature extraction** (**FE**)
- **Blind source separation** (**BSS**)
- Detection of **anomalies** / disruptions
- Separate concurring processes
- Discover unknown processes, dependencies and phenomena hidden the data
- Identify dependencies between model inputs and outputs
- Develop **reduced-order models**
- **“Label” datasets** for supervised ML analyses

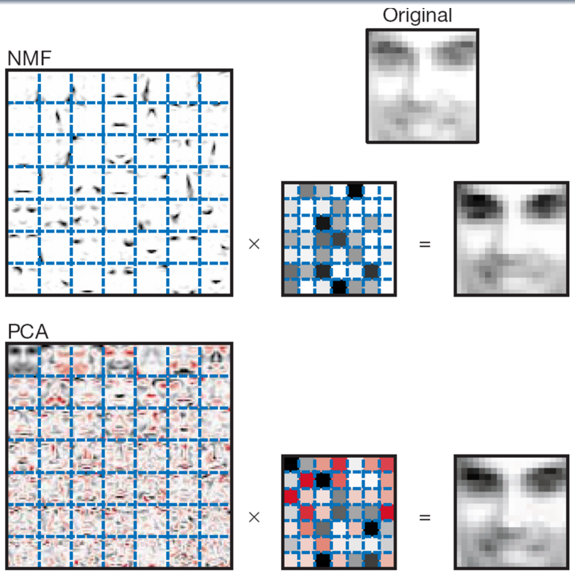
Nonnegative Matrix/Tensor Factorization

- Novel LANL-patented, open-source, unsupervised Machine Learning (ML) methods
- Matrix/Tensor Factorization coupled with custom k-means clustering and nonnegativity/sparsity constraints:
  - NMFk: Nonnegative **Matrix** Factorization
  - NTFk: Nonnegative **Tensor** Factorization
- Allowing for data gaps
- Reconstructing missing data
- Efficient processing of large datasets (TB's) utilizing GPU's, TPU's & FPGA's
- julia: as **fast** as C/FORTRAN; as **easy** as MATLAB/Python

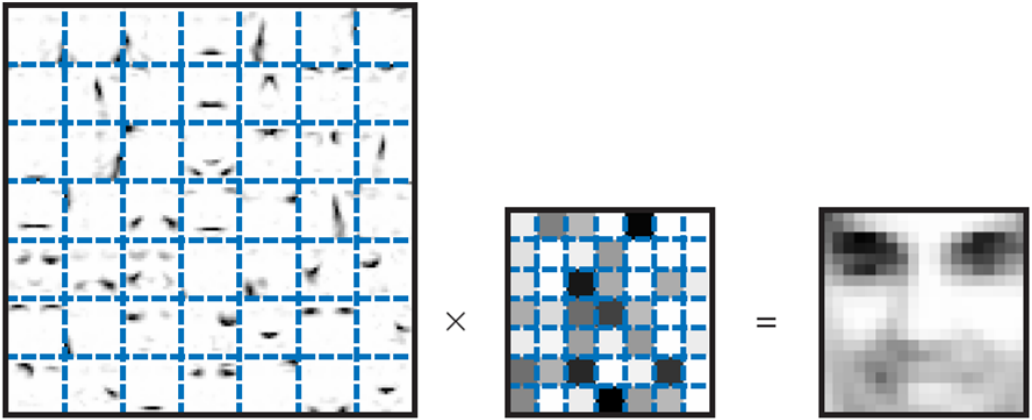




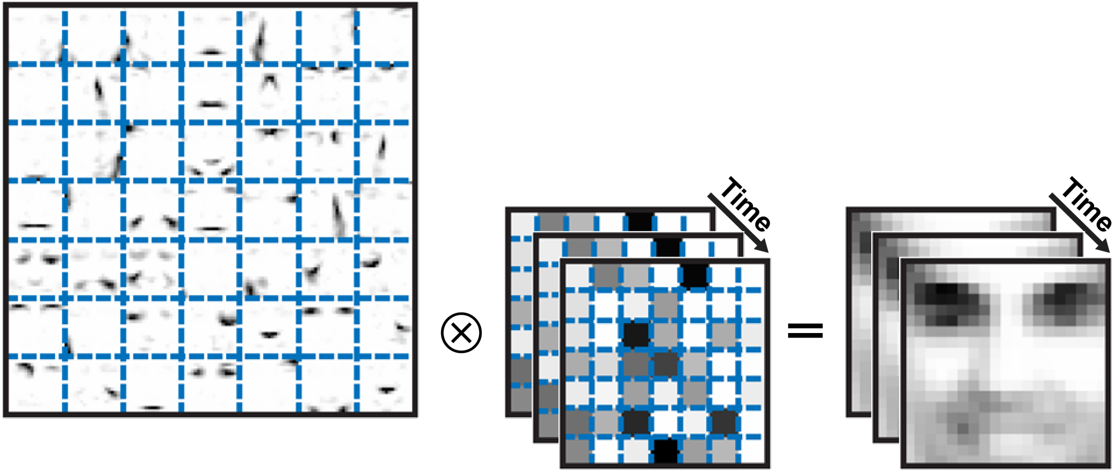
- **NMF** vs **PCA** (Lee & Seung, Nature, 1999)
- **NMF**: Nonnegative Matrix Factorization
- **PCA**: Principal Component Analysis
- **Nonnegativity** constraints provide **meaningful** and **interpretable** results (+**sparsity**)



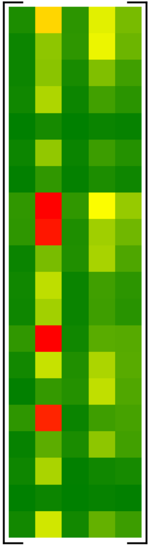
NMF: Nonnegative Matrix Factorization



NTF: Nonnegative Tensor Factorization



NMFk: data matrix



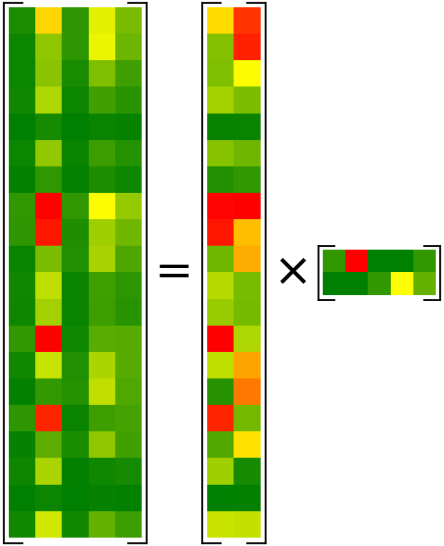
$\boldsymbol{X}$

$[20 \times 5]$

$\boldsymbol{X}$ – **data** matrix

$[$**attributes** $\times$ **observations**$]$

NMFk: matrix factorization



$$\boldsymbol{X} = \boldsymbol{W} \times \boldsymbol{H}$$

$$[20 \times 5] = [20 \times 2] \times [2 \times 5]$$

$\boldsymbol{X}$ – **data** matrix

[**attributes** $\times$ **observations**]

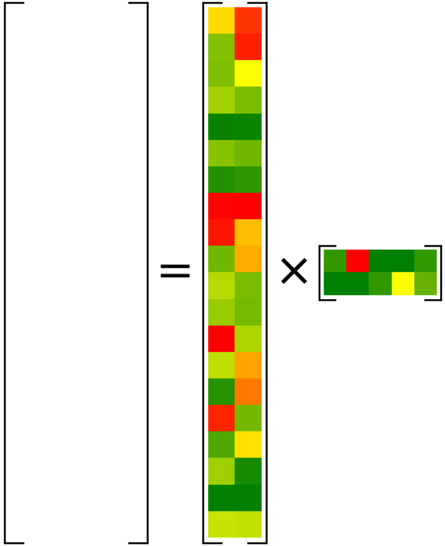
$\boldsymbol{W}$ – **feature** (**signal**) matrix

[**attributes** $\times$ **features**]

$\boldsymbol{H}$ – **mixing** matrix

[**features** $\times$ **observations**]

NMFk: true matrix factors



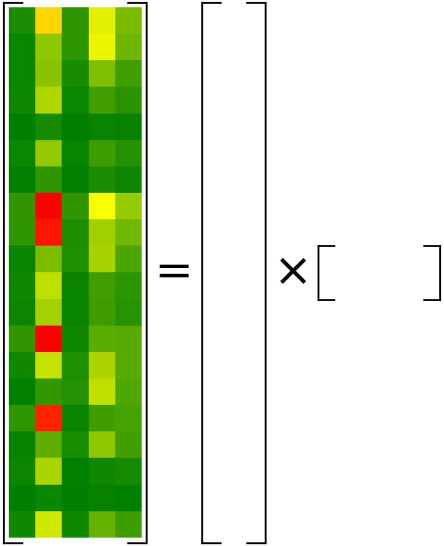
$$\boldsymbol{X} = \boldsymbol{W} \times \boldsymbol{H}$$
$$[20 \times 5] = [20 \times 2] \times [2 \times 5]$$

$\boldsymbol{X}$ – **data** matrix
[**attributes** $\times$ **observations**]

$\boldsymbol{W}$ – **feature** (**signal**) matrix
[**attributes** $\times$ **features**]

$\boldsymbol{H}$ – **mixing** matrix
[**features** $\times$ **observations**]

NMFk: true data matrix



$$\boldsymbol{X} = \boldsymbol{W} \times \boldsymbol{H}$$

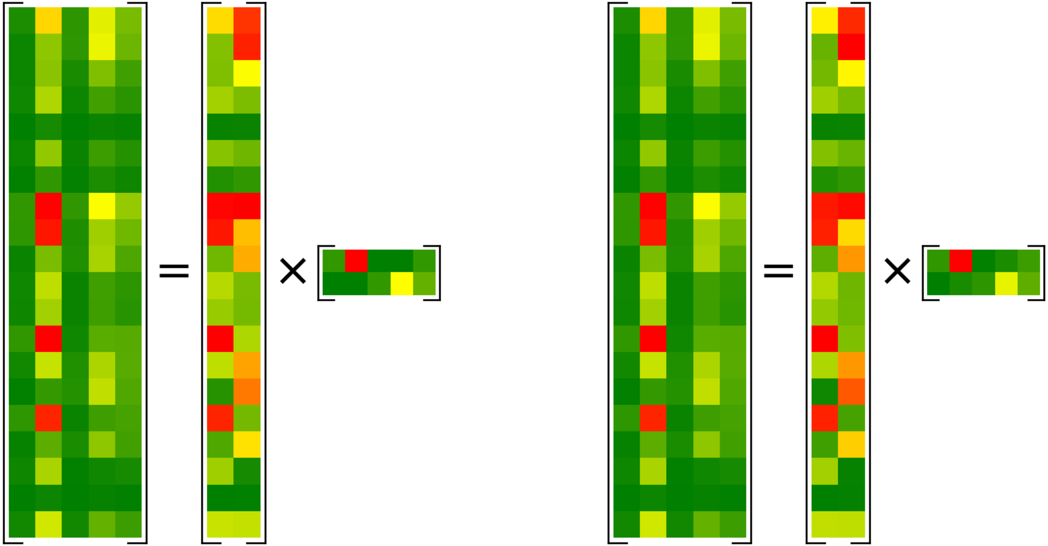
$$[20 \times 5] = [20 \times \textbf{?}] \times [\textbf{?} \times 5]$$

$\Rightarrow$ 100 **knowns**

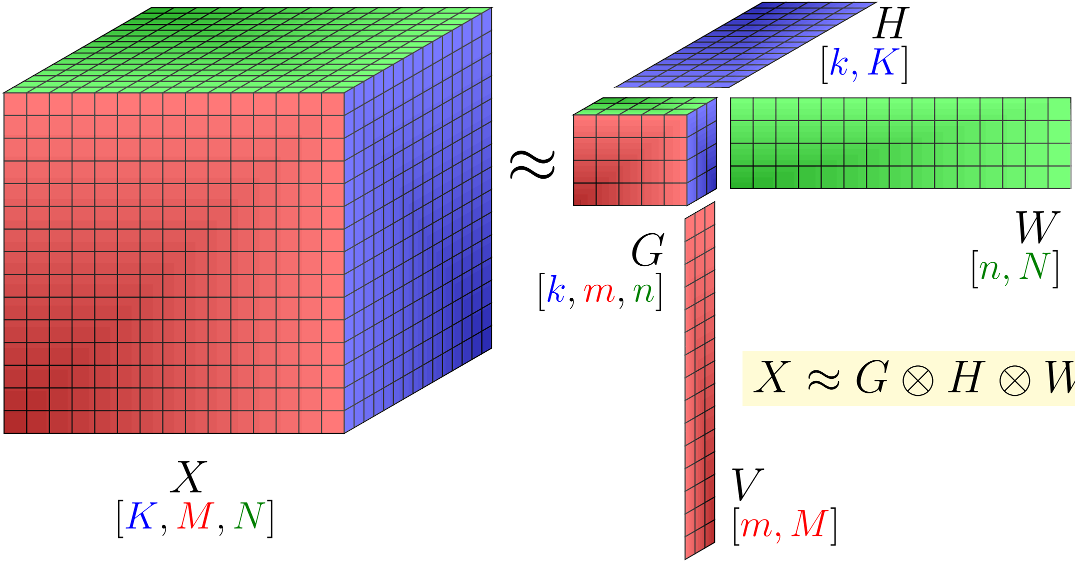
$\Rightarrow$ **unknown** number of features (2 or more)

$\Rightarrow$ **unknown** matrix elements of $\boldsymbol{W}$ and $\boldsymbol{H}$ (50 or more)

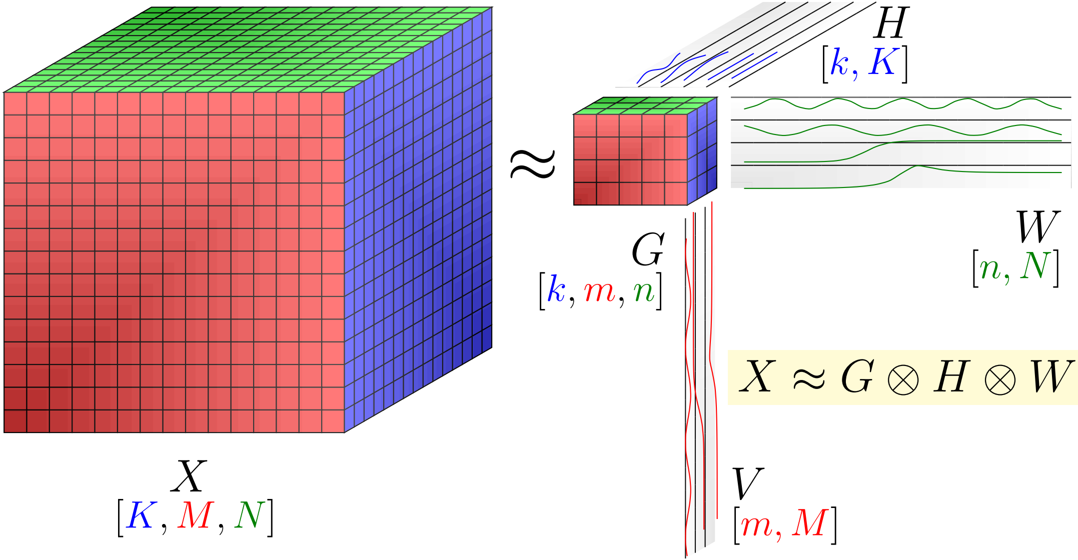
NMFk: true vs. estimated matrix factorization



NTFk: Tensor Decomposition

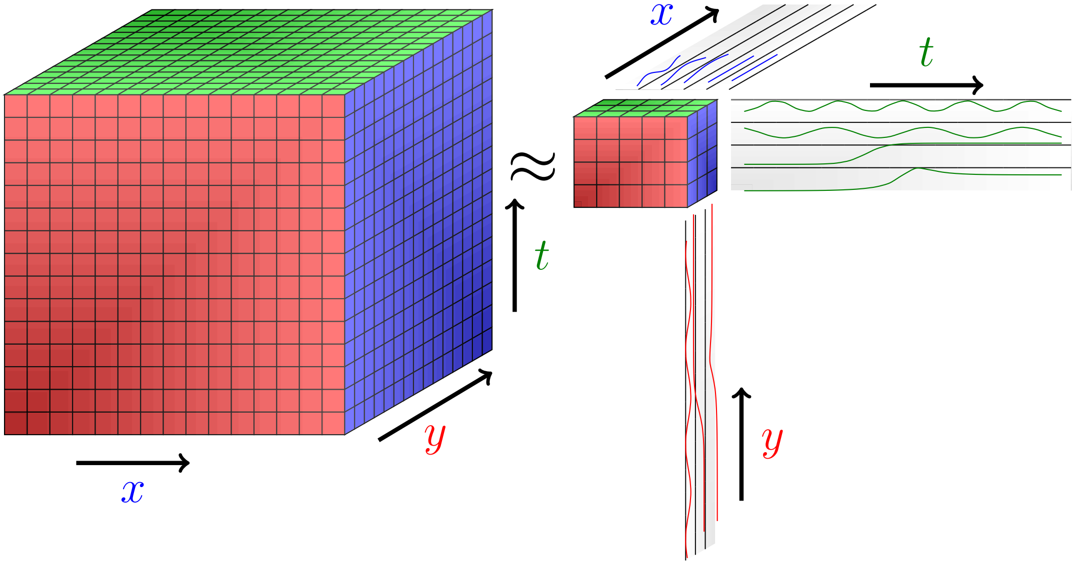


$$X \approx G \otimes H \otimes W \otimes V$$



$$X \approx G \otimes H \otimes W \otimes V$$

NTFk: Tensor Decomposition: Feature extraction



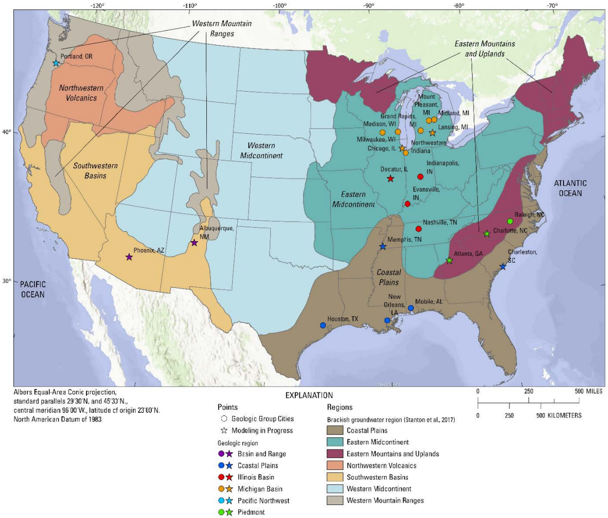
NMFk / NTFk Analyses

- **Field Data**:
  - Contamination
  - Climate
  - Geothermal
  - Seismic
  - Oil/gas production
- **Lab Data**:
  - X-ray Spectroscopy
  - UV Fluorescence Spectroscopy
  - Microbial populations
  - Isotope fractionation
- **Operational Data**:
  - LANSCE: Los Alamos Neutron Accelerator
  - Oil/gas production
- **Modeling Results**:
  - Reactive mixing $A + B \rightarrow C$
  - Phase separation of co-polymers
  - Molecular Dynamics of proteins
  - Climate

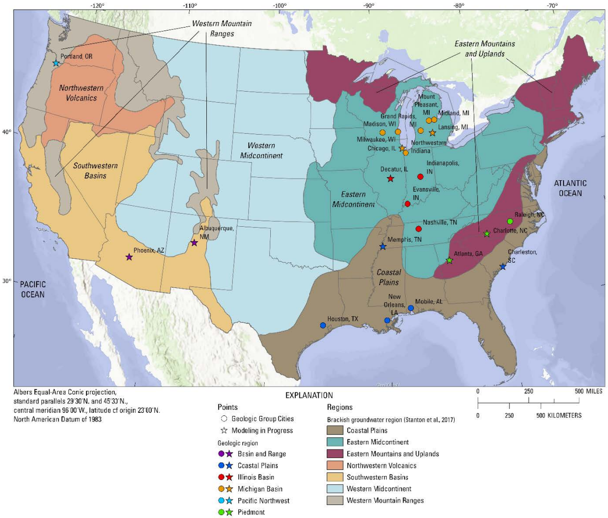
NMFk / NTFk Publications

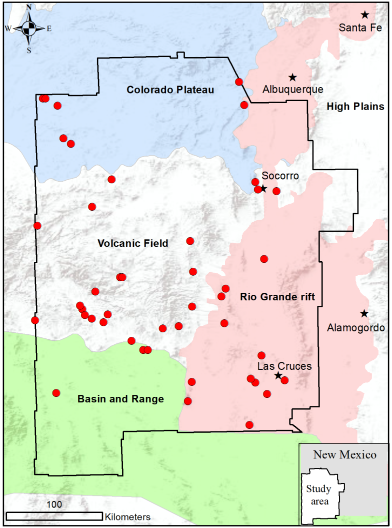
- Vesselinov, Munuduru, Karra, O'Maley, Alexandrov, Unsupervised Machine Learning Based on Non-Negative Tensor Factorization for Analyzing Reactive-Mixing, **Journal of Computational Physics**, Special issue: Machine Learning, 2019.
- Stanev, Vesselinov, Kusne, Antoszewski, Takeuchi, Alexandrov, Unsupervised Phase Mapping of X-ray Diffraction Data by Nonnegative Matrix Factorization Integrated with Custom Clustering, **Nature Computational Materials**, 2018.
- Vesselinov, O'Malley, Alexandrov, Nonnegative Tensor Factorization for Contaminant Source Identification, **Journal of Contaminant Hydrology**, 2018.
- O'Malley, Vesselinov, Alexandrov, Alexandrov, Nonnegative/binary matrix factorization with a D-Wave quantum annealer, **PLOS ONE**, 2018.
- Vesselinov, O'Malley, Alexandrov, Contaminant source identification using semi-supervised machine learning, **Journal of Contaminant Hydrology**, 2017.
- Alexandrov, Vesselinov, Blind source separation for groundwater level analysis based on nonnegative matrix factorization, **WRR**, 2014.

Geothermal: New Mexico: Study Area



Geothermal: New Mexico: Study Area





Geothermal: New Mexico: Data

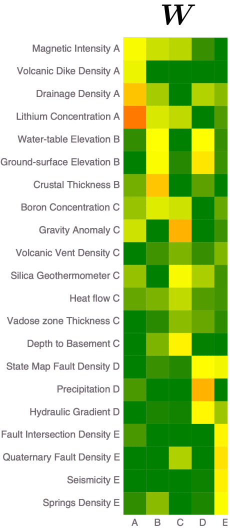
X^T $[44 \times 21]$
[locations $\times$ attributes]

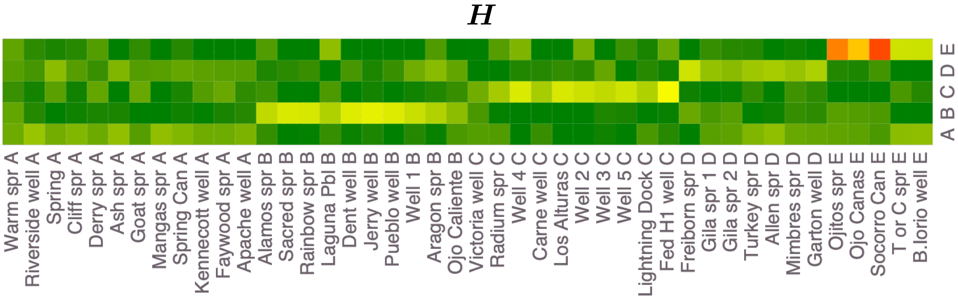
- Boron Concentration
- Gravity Anomaly
- Magnetic Intensity
- Volcanic Dike Density
- Drainage Density
- Fault Intersection Density
- Quaternary Fault Density
- Seismicity
- State Map Fault Density
- Springs Density
- Volcanic Vent Density
- Lithium Concentration
- Precipitation
- Silica Geothermometer Temp
- Hydraulic Gradient
- Watertable Elevation
- Heat flow
- Elevation
- Watertable Depth
- Crust Thickness
- Depth to Basement

[Pepin, 2019]

Location	Boron	Gravity	Magnet	Dikes	Drain	Fault	Qfault	Seism	NMFlt	Springs	Vents	Lithium	Precip	Silica	Δh	WT	Qheat	Elev	DTW	Crust	Bsmt
Alamos Spring	-0.2	-203.3	136.2	0.431	7.4	0.000	0.00	0.004	16.2	0.010	0.003	-3.1	264.8	16.5	5.6	5812	4.6	1763	-21.5	38.7	1439
Allen Springs	-3.2	-189.3	184.6	3.625	17.3	0.000	0.01	0.002	15.6	0.003	0.001	-4.0	514.5	24.0	13.9	5994	4.4	1805	-20.1	32.5	51
Apache Tejo Warm Springs well	-1.8	-181.2	15.0	3.807	17.3	0.001	0.03	0.001	0.7	0.003	0.000	-8.6	326.3	52.0	4.7	5261	4.6	1641	34.6	30.7	24
Aragon Springs	1.5	-229.1	-317.7	0.010	19.0	0.000	0.00	0.000	41.1	0.005	0.003	-7.5	387.0	56.5	4.0	6981	4.5	2094	-30.1	38.8	1486
Ash Spring	-2.7	-193.2	66.6	4.914	17.0	0.000	0.00	0.002	9.3	0.003	0.000	-5.0	492.0	29.3	4.1	5712	4.4	1806	71.9	32.2	-92
B. Iorio 1 well	-2.1	-196.5	-48.2	1.936	18.8	0.057	21.02	0.000	9.1	0.003	0.003	-2.6	260.4	59.4	0.9	4240	4.0	1298	7.7	30.9	-188
Cliff Warm Spring	-2.5	-199.1	-47.1	1.290	22.8	0.001	2.58	0.002	11.0	0.002	0.001	-6.9	364.2	64.2	1.8	4546	4.2	1378	-6.7	33.1	-191
Dent windmill well	-2.1	-230.8	89.3	0.000	13.4	0.000	0.00	0.000	0.0	0.005	0.000	-7.3	341.7	19.7	2.4	6600	4.7	2108	94.3	43.5	865
Derry Warm Springs	-1.5	-161.6	197.0	0.659	18.3	0.007	9.16	0.000	15.9	0.002	0.000	-7.5	276.1	37.4	3.0	4183	4.6	1391	130.5	30.0	-120
Faywood Hot Springs	-2.6	-172.1	-49.8	0.939	16.6	0.002	2.81	0.000	1.9	0.003	0.000	-4.8	346.4	67.2	4.2	4910	5.5	1548	49.6	30.0	619
Federal H 1 well	-0.4	-132.0	35.0	0.000	5.8	0.004	20.31	0.001	7.2	0.000	0.015	-5.0	253.8	78.7	2.7	4104	4.9	1315	68.1	27.3	2906
Freiborn Canyon Spring	-2.5	-225.0	-242.0	0.401	13.1	0.000	0.00	0.001	19.8	0.001	0.004	-12.6	538.6	49.8	13.0	7123	4.6	2207	30.9	38.4	1138
Garton well	-3.2	-196.8	35.6	0.150	18.0	0.000	0.00	0.000	28.9	0.002	0.001	-5.0	489.9	70.0	4.3	6165	3.9	2037	146.4	30.9	-266
Gila Hot Springs 1	-1.9	-221.6	-149.3	0.127	24.2	0.000	0.00	0.001	25.5	0.003	0.003	-7.8	422.6	69.9	6.6	5867	4.4	1773	-25.7	34.0	413
Gila Hot Springs 2	-1.8	-222.9	-138.8	0.112	24.7	0.000	0.00	0.001	23.7	0.003	0.003	-6.7	425.9	70.8	3.2	5921	4.6	1811	-1.5	33.9	519
Goat Camp Spring	-2.1	-159.2	-29.7	0.751	10.0	0.001	2.22	0.007	10.6	0.002	0.001	-8.0	344.0	68.9	5.8	4480	4.4	1357	5.8	32.4	19
Jerry well	-0.8	-219.6	172.4	0.111	15.5	0.000	0.00	0.000	6.3	0.004	0.005	-7.9	243.9	13.4	1.0	6360	4.4	1947	6.3	42.3	1190
Kennecott Warm Springs well	-2.4	-178.3	-69.9	1.422	17.8	0.002	1.76	0.000	1.1	0.003	0.000	-6.9	355.0	66.1	4.3	4890	5.0	1520	28.9	30.0	409
Laguna Pueblo	0.4	-204.2	62.5	0.406	8.6	0.004	4.58	0.006	14.6	0.018	0.005	-3.3	259.7	42.9	2.6	5364	4.4	1628	-13.5	37.2	1506
Lightning Dock	-1.0	-168.0	-168.1	0.086	4.6	0.008	8.40	0.002	4.3	0.000	0.000	-3.9	291.5	107.3	0.8	4147	5.0	1278	14.3	29.8	1800
Los Alturas Estates	-1.5	-141.4	-127.5	0.004	7.6	0.003	0.05	0.002	6.6	0.001	0.000	-12.7	265.3	71.9	2.2	3892	6.3	1279	102.9	27.4	4321
Mangas Springs	-2.6	-201.0	-227.1	3.503	20.2	0.000	0.91	0.002	11.5	0.002	0.000	-4.5	393.5	53.6	0.3	4784	4.2	1459	-5.0	32.4	-178
Mimbres Hot Springs	-2.3	-200.6	43.4	0.670	15.4	0.002	1.13	0.000	19.0	0.004	0.000	-3.8	445.9	68.3	9.1	5914	4.9	1834	66.4	31.0	50
Ojitos Springs	-1.6	-202.1	-7.5	1.342	19.6	0.044	19.74	0.037	31.0	0.020	0.005	-4.5	257.5	57.6	7.2	5227	4.5	1594	2.3	33.0	-255
Ojo Caliente	-2.6	-226.5	-168.4	0.000	20.5	0.000	0.00	0.000	8.3	0.004	0.000	-2.9	333.6	48.4	3.5	6263	5.5	1987	74.0	33.8	2415
Ojo De las Canas	-1.7	-188.5	-85.8	0.839	22.3	0.036	12.55	0.036	28.0	0.013	0.003	-6.0	270.5	14.2	4.0	5003	4.5	1585	54.7	31.8	101
Pueblo windmill well	-1.2	-228.8	315.9	0.029	15.2	0.000	0.00	0.000	6.1	0.004	0.003	-12.0	265.8	18.3	2.9	6419	4.3	1963	6.0	42.5	1027
Radium Hot Springs	-0.8	-151.4	-7.8	0.010	8.8	0.013	11.40	0.003	10.6	0.001	0.000	-5.3	264.2	63.6	0.3	3982	5.4	1229	24.4	28.2	1191
Rainbow Spring	-1.7	-227.1	-48.5	0.000	11.0	0.000	0.00	0.001	0.0	0.006	0.000	-7.0	307.8	21.7	3.3	6269	4.7	1955	52.0	43.9	755
Riverside Store well	-1.3	-196.1	-102.9	1.562	22.6	0.000	2.50	0.002	11.7	0.002	0.001	-2.4	356.1	60.8	0.9	4489	4.3	1368	2.8	32.9	-165
Sacred Spring	-1.8	-228.4	-80.4	0.000	10.9	0.000	0.00	0.001	0.0	0.006	0.000	-7.0	298.4	21.2	1.3	6271	4.6	1940	29.7	43.9	742
Socorro Canyon	-1.8	-204.7	-136.5	1.203	21.1	0.051	28.88	0.034	33.8	0.020	0.005	-6.7	284.1	44.6	11.1	5237	5.0	1692	67.7	32.6	-229
Spring	-4.1	-183.5	334.5	0.218	20.1	0.011	1.81	0.000	20.1	0.001	0.006	-6.8	361.9	117.2	5.1	5472	3.8	1759	88.1	31.5	-104
Spring Canyon Warm Spring	-2.1	-194.2	117.3	2.293	21.9	0.000	1.50	0.002	12.7	0.002	0.000	-8.3	361.7	51.6	5.8	4576	4.2	1457	60.2	32.6	-57
Truth or Consequences spring	-1.1	-168.2	-54.3	2.175	18.4	0.064	20.51	0.000	10.3	0.003	0.002	-3.3	265.9	55.3	0.6	4255	4.3	1293	-8.4	31.0	304
Turkey Creek Spring	-3.2	-196.4	54.8	0.984	19.2	0.001	3.69	0.002	28.1	0.002	0.002	-3.7	493.4	81.3	5.8	5478	4.4	1718	7.7	33.6	56
Victoria Land and Cattle Co. well	-1.8	-165.9	-65.4	0.478	6.4	0.003	0.06	0.001	0.9	0.001	0.000	-2.9	253.0	43.0	1.9	4762	4.1	1461	9.6	30.7	2014
Warm Springs	-2.1	-193.3	113.5	0.220	19.0	0.029	2.63	0.000	16.5	0.004	0.003	-2.5	314.6	56.0	5.4	5777	4.3	1797	-1.7	32.7	1252
Well 1	-1.4	-230.7	-31.3	1.190	15.7	0.000	0.75	0.001	22.1	0.004	0.002	-6.6	345.4	49.0	1.7	7382	4.4	2249	1.8	40.0	1961
Well 2	-1.2	-162.5	0.8	0.000	4.5	0.008	24.24	0.003	11.8	0.000	0.006	-10.1	279.5	70.5	1.7	4291	4.8	1355	49.7	27.8	2993
Well 3	-2.5	-140.0	31.7	0.839	2.1	0.001	2.11	0.001	5.0	0.001	0.000	-7.3	369.0	51.0	4.1	4765	4.3	1907	431.7	28.0	3073
Well 4	-1.3	-161.7	-56.1	0.000	3.4	0.008	28.49	0.003	10.6	0.000	0.006	-10.0	274.3	94.0	1.9	4082	4.7	1338	91.3	27.7	3373
Well 5	-1.9	-167.2	-29.9	0.000	2.5	0.008	15.48	0.002	3.1	0.000	0.005	-6.8	243.8	47.0	0.3	3839	4.0	1276	106.1	27.4	5460
Well south of Carne	-2.4	-156.7	-129.6	0.457	4.3	0.000	2.11	0.002	6.0	0.001	0.000	-6.8	269.7	87.1	1.4	4109	4.5	1275	13.5	28.4	2761

Geothermal: New Mexico: NMFk Results



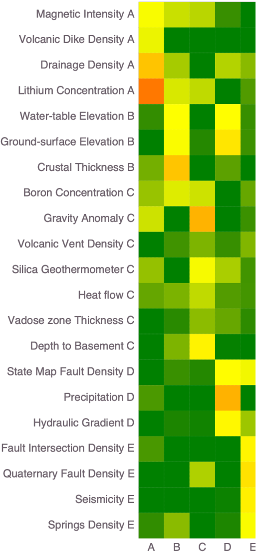


$$X = W \times H$$

5 signatures extracted (A, B, C, D, E)

W: mapping of the **signatures** to geothermal **attributes**

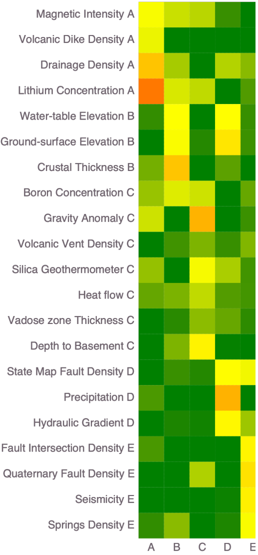
H: mapping of the **signatures** to geothermal **locations**



Dominant signature attributes:

- **Signature C**
  - Volcanic Vent Density
  - Gravity Anomaly
  - Heat flow
  - Silica Geothermometer
  - Watertable Depth
  - Depth to Basement
  - Boron
- **Signature A**
  - Volcanic Dike Density
  - Magnetic Intensity
  - Drainage Density
  - Lithium
- **Signature B**
  - Water-table Elevation
  - Ground-surface Elevation
  - Crust Thickness
- **Signature D**
  - Precipitation
  - Hydraulic Gradient
  - State Map Fault Density
- **Signature E**
  - Seismicity
  - Fault Intersection Density
  - Quaternary Fault Density
  - Springs Density

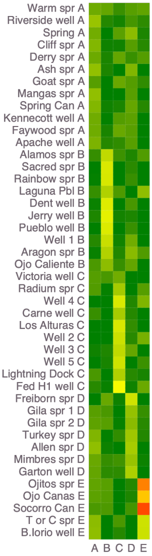
Geothermal: New Mexico: NMFk Results

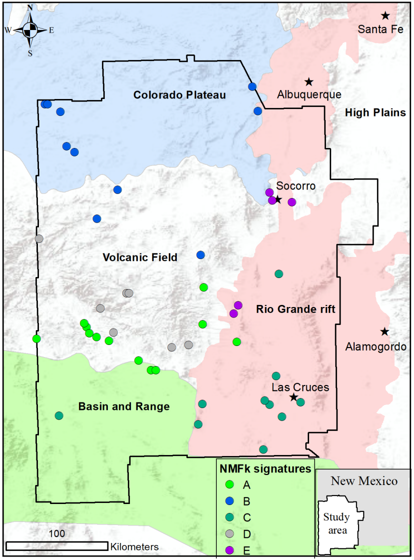


Physics interpretation:

- **Signature C: Deep heat flow**
  - Volcanic Vent Density
  - Gravity Anomaly
  - Heat flow
  - Silica Geothermometer
  - Watertable Depth
  - Depth to Basement
  - Boron
- **Signature A: Shallow heat flow**
  - Volcanic Dike Density
  - Magnetic Intensity
  - Drainage Density
  - Lithium
- **Signature B: Lateral hydraulics**
  - Water-table Elevation
  - Ground-surface Elevation
  - Crust Thickness
- **Signature D: Vertical hydraulics**
  - Precipitation
  - Hydraulic Gradient
  - State Map Fault Density
- **Signature E: Tectonics**
  - Seismicity
  - Fault Intersection Density
  - Quaternary Fault Density
  - Springs Density

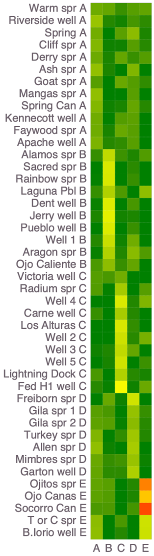
Geothermal: New Mexico: NMFk Results

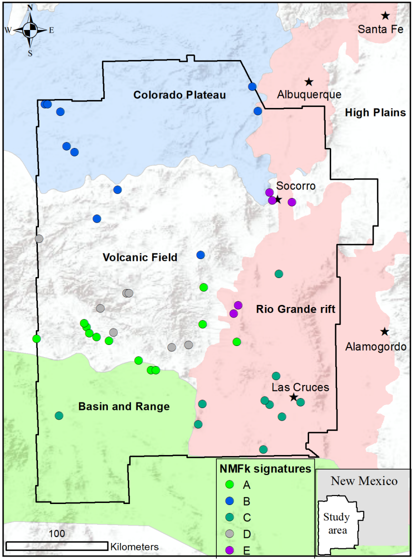




Province association:

- Signature A:
  Colorado Plateau
- Signature B:
  Basin and Range
- Signature C:
  Volcanic Field #1
- Signature D:
  Volcanic Field #2
- Signature E:
  Rift Zone





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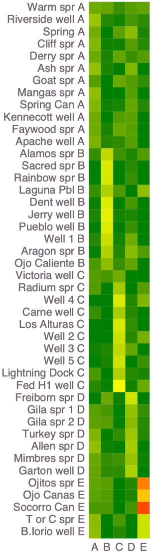
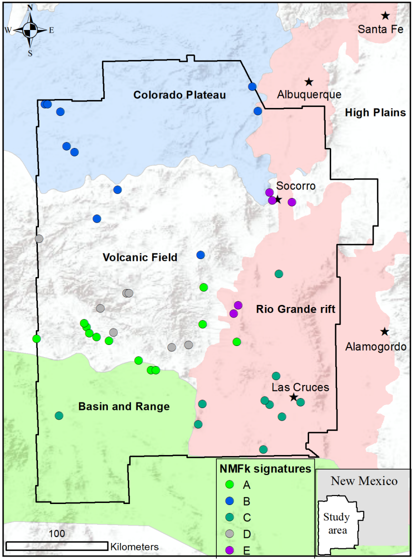
Geothermal: New Mexico: NMFk Results



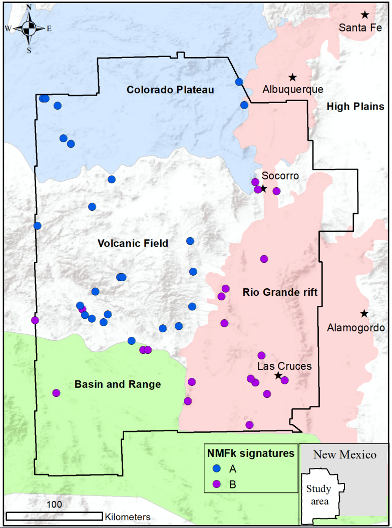


Physics/province association:

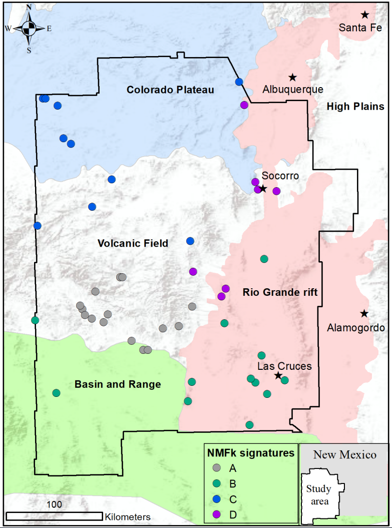
- Signature A:
  Colorado Plateau ⇔ **Shallow heat flow**
- Signature B:
  Basin and Range ⇔ **Lateral hydraulics**
- Signature C:
  Volcanic Field #1 ⇔ **Deep heat flow**
- Signature D:
  Volcanic Field #2 ⇔ **Vertical hydraulics**
- Signature E:
  Rift Zone ⇔ **Tectonics**

Geothermal: New Mexico: NMFk Results

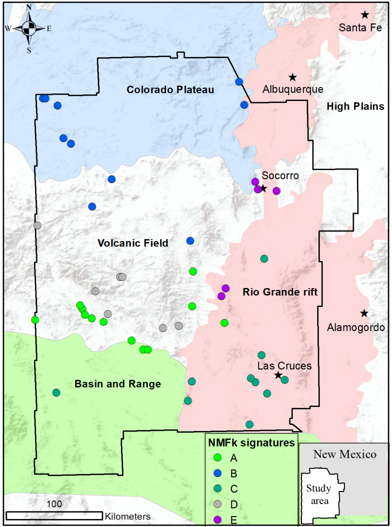
2 signatures



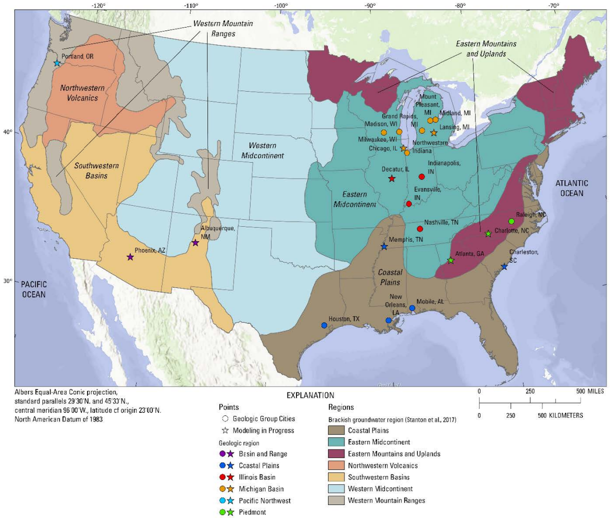
4 signatures

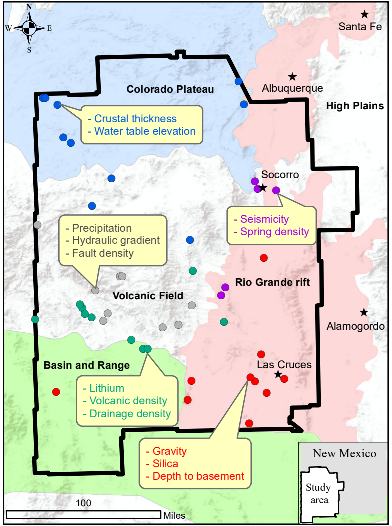


5 signatures

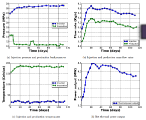


Geothermal: New Mexico: NMFk Results





Geothermal: ML workflow

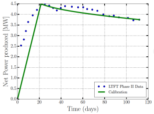


1. Process site data:
- Permeability, Porosity
- Pressure, Diffusivity
- Thermal conductivity
- Heat/mass flux
- Chemical species, etc.

2. Estimate spatially distributed THC model parameters

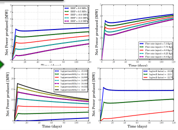
3. Generate THC model parameters and inputs

4. Simulate 3D high-resolution multi-physics heat/mass flow and species transport (PFLOTRAN/E4D/dfnWorks/REALMS)



5. Calibrate and compare with site-/regional-scale field data

6. Estimate sensitivity of model inputs



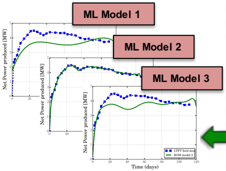
7. Identify key THC model parameters

8. Key parameters: Fractured rock permeability, heat flux, injection mass flow rate, etc.

9. Select key THC parameters/inputs

10. Create Machine Learning (ML) models

11. Compare ML models with test data and make prediction on field-data



ML Model 1

$$Power_{\text{rom-1}} = a_0(t) + \sum_{i=1}^{3} b_i(t)\left(|\log(k_{\text{fz}})| + 10^{-6}t\right)^i$$

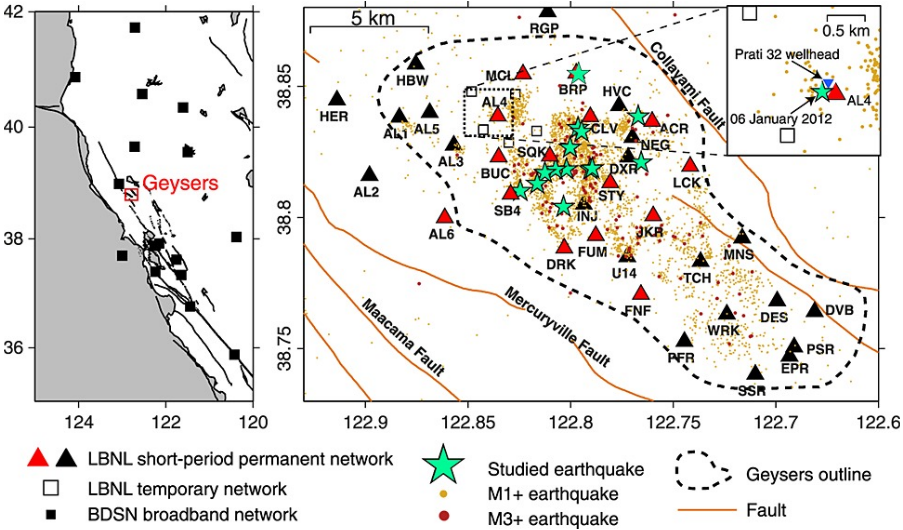
ML Model 2

$$Power_{\text{rom-2}} = b_0(t) + \sum_{i=1}^{3} b_i(t)\left(|\log(k_{\text{fz}})| + 10^{-6}t\right)^i + \underbrace{\sum_{j=1}^{29} m_j\left(1 + \tanh(n_j(t - t_j))\right)^{r_j}}_{\text{Smooth approximation of Heaviside function}}$$

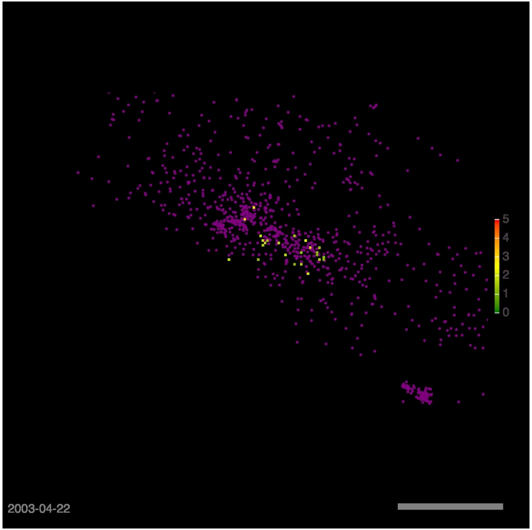
ML Model 3

$$Power_{\text{rom-3}} = c_0(t) + \sum_{i=1}^{3} c_i(t)\left(|\log(k_{\text{fz}})| + 10^{-6}t\right)^i$$

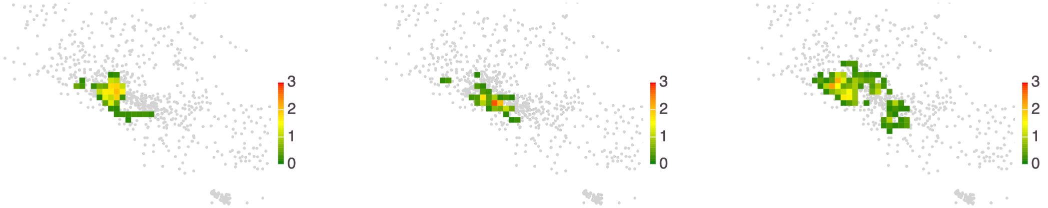
Geysers Geothermal Field

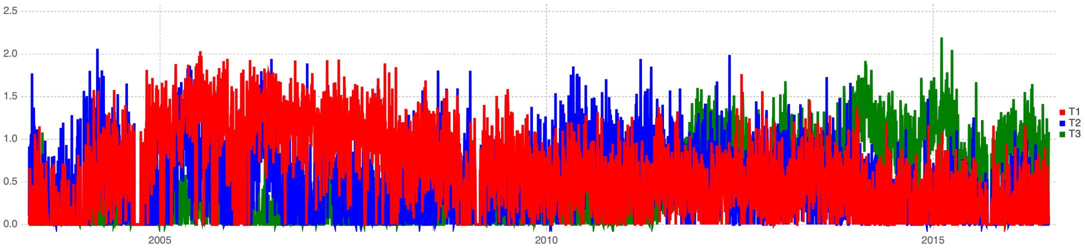


- 470,263 seismic events have been identified between 2003 and 2016
- Tensor: total energy of events over a discretized domain
- **NTFk** extracts spatial footprints and temporal patterns of dominant hidden (latent) features related to:
  - Total water injection
  - EGS injection (starting November 6th, 2011)
  - ...

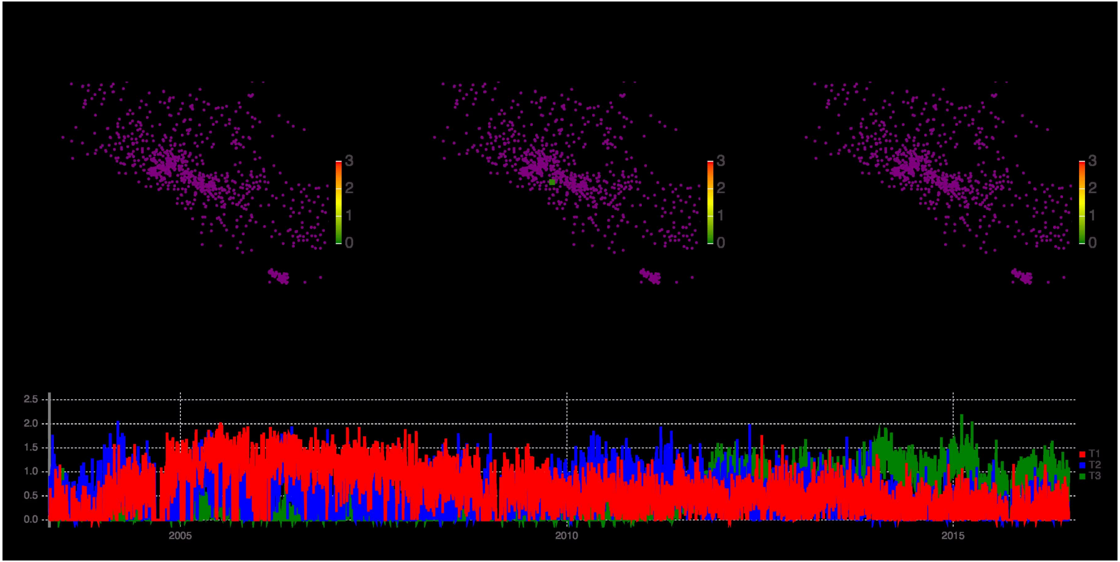


Geysers seismicity: NTFk results

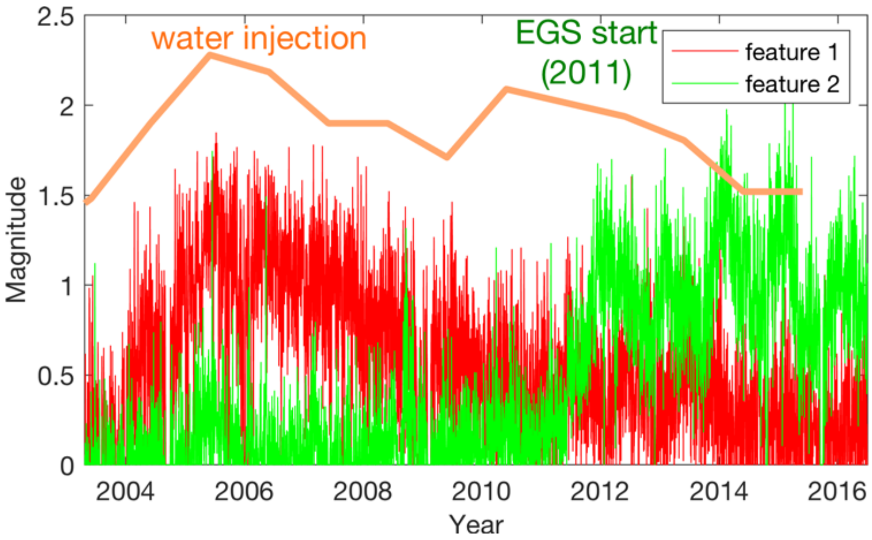




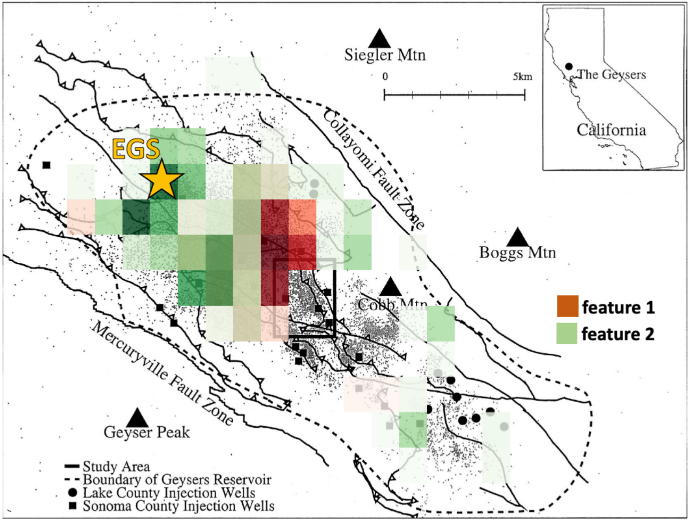
Geysers seismicity: NTFk results



Geysers seismicity: NTFk results



Geysers seismicity: NTFk results



Summary

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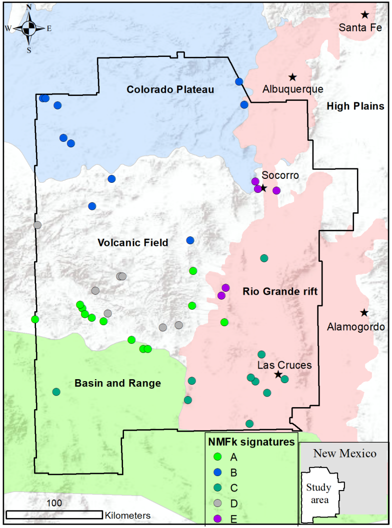
Our novel ML methods (**NMF*k*/NTF*k***) have been successfully applied to **extract features** characterizing :

- Geothermal data collected in Southwestern New Mexico
- Seismic activity at the Geysers Geothermal Field, California

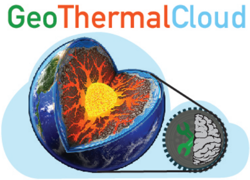
NMF*k*/NTF*k* s will be also applied to other LANL geothermal work:

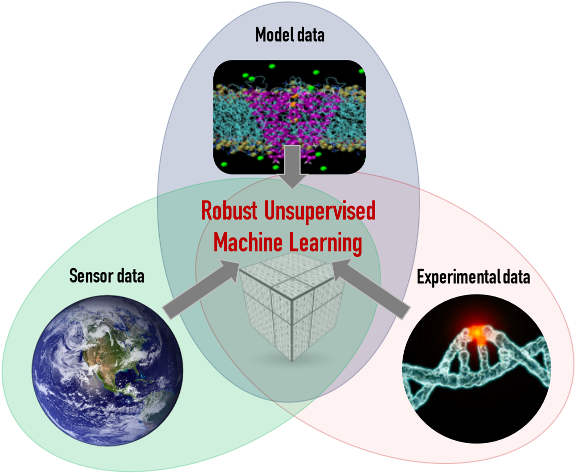
- Laboratory experiments related to fracture caging (**Frash et al.**)
- Simulations of the 3D geothermal heat flow in fractured media (**Makedonska et al.**, **Jafarov et al.**)



Summary

- Developed **novel unsupervised** and **physics-informed** ML methods and computational tools
- Our ML methods have been already applied to solve various real-world problems
- julia: as **fast** as C/FORTRAN; as **easy** as MATLAB/Python





Machine Learning (ML) Algorithms / Codes developed by our team

- Open-source codes:

NMFk MADS NTFk

- Scripts, examples, tests, Jupyter notebooks, Docker images:

```
http://tensors.lanl.gov
http://tensordecompositions.github.io
https://github.com/TensorDecompositions
http://madsjulia.github.io/Mads.jl/Examples/blind_source_separation
https://hub.docker.com/u/montyvesselinov
```